INTERACTION OF MOVING BREATHERS WITH AN IMPURITY

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We analyze the influence of an impurity in the evolution of moving discrete breathers in a Klein–Gordon chain with non-weak nonlinearity. Three different behaviours can be observed when moving breathers interact with the impurity: they pass through the impurity continuing their direction of movement; they are reflected by the impurity; they are trapped by the impurity, giving rise to chaotic breathers. Resonance with a breather centred at the impurity site is conjectured to be a necessary condition for the appearance of the trapping phenomenon.

1. Introduction

The interaction of nonlinear localized oscillations with impurities in a system can play an important role in its transport properties. This problem has been studied during the last decades within different frameworks, e.g. the scattering of kinks with impurities in the continuous sine-Gordon and ϕ^4 models [1] and in the Frenkel–Kontorova model [2]. The interaction of a moving discrete breather with an impurity in a Klein–Gordon chain has been considered by Forinash et al [3]. In this case, it is assumed that the system has weak nonlinearity. Here, we are interested in the study of the features of the interaction of moving discrete breathers with an impurity at rest in a Klein–Gordon chain of oscillators with non-weak nonlinearity. We also establish a hypothesis for the appearance of trapping of a breather by an impurity.

2. The Model

We consider a Klein–Gordon chain with nearest neighbours attractive interactions with Hamiltonian given by:

$$H = \sum_{n=1}^{N} \left(\frac{1}{2}\dot{u}_n^2 + V_n(u_n) + \frac{1}{2}C(u_n - u_{n-1})^2 \right), \tag{1}$$

where $V_n(u_n) = D_n(e^{-u_n} - 1)^2$ is the substrate potential at the n-th site. The inhomogeneity is introduced assuming a different well depth at only one site, i.e., $D_n = D_o(1 + \alpha\delta_{n,0})$, then we refer to the particle located at $n = 0$ as an impurity. $\alpha \in [-1,\infty)$ is a parameter which tunes the magnitude of the inhomogeneity.

This Hamiltonian leads to the dynamical equations which have stationary and moving localized solutions (i.e., stationary and moving breathers). The former are calculated using the methods based in the anti–continuous limit [5] and the latter are calculated using the marginal mode method [4].

The dynamical equations can be linearized if the amplitudes of the oscillations are small. These equations have $N - 1$ non-localized solutions (*linear extended modes*) and one localized solution, (*linear impurity mode*). Their frequencies, ω_E and ω_L, respectively, are given by:

$$\omega(q,\alpha) = \sqrt{\omega_o^2 + 4C\sin^2\frac{q(\alpha)}{2}}, \quad \omega_L^2 = \omega_o^2 + 2C + \mathrm{sign}(\alpha)\sqrt{\alpha^2\omega_o^4 + 4C^2}, \tag{2}$$

where $q \in (0,\pi]$ if $\alpha < 0$ and $q \in [0,\pi)$ if $\alpha > 0$. Figure 1 shows the dependence on α.

3. Numerical simulations

We have studied the behaviour of moving breathers when they interact with an impurity varying the value of the inhomogeneity parameter α. We have found four different regimes, separated by critical values of the parameter α [6]:

- *Barrier.* The impurity acts as a potential barrier. It occurs either with $\alpha > 0$ or $\alpha \in (-1,\alpha_1)$ with $\alpha_1 < 0$. If $\alpha \gtrsim 0$, the breather can pass through the impurity provided the translational velocity is high enough [7].
- *Excitation.* The impurity is excited and the breather is reflected. It occurs for $\alpha \in (\alpha_1,\alpha_2)$. This behavior is shown in figure 2.
- *Trapping.* The breather is trapped by the impurity. It occurs in the interval $\alpha \in (\alpha_2,\alpha_3)$. When the moving breather is close to the impurity, it becomes trapped while its center oscillates between the
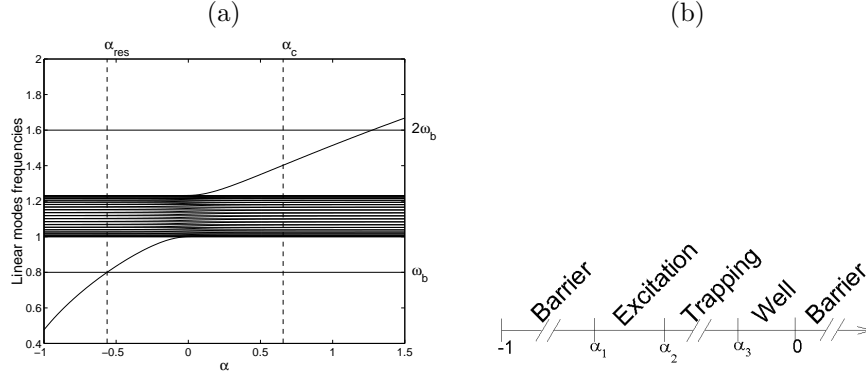
(a) (b)

Figure 1. (a) Frequencies of the linear modes versus the parameter α. At $\alpha = \alpha_{res}$ and $\alpha = \alpha_c$, two different bifurcations occur, being the first one due to the resonance between the impurity mode and the breather. (b) Different regimes in the interaction of a moving breather with an impurity introduced as an inhomogeneity in the potential well depth.
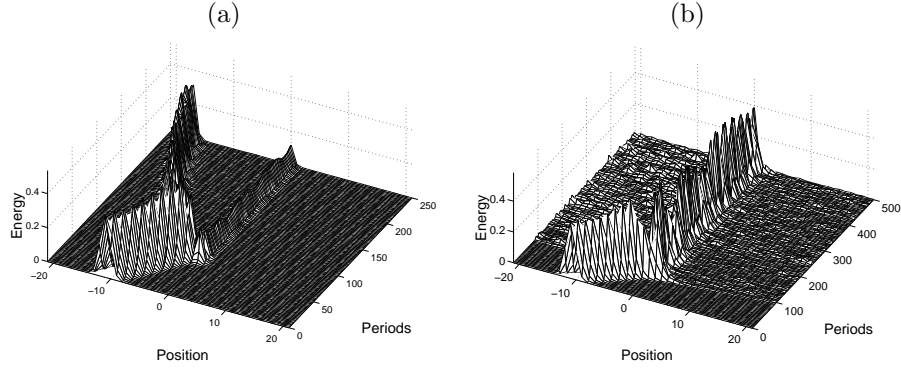
(a) (b)

Figure 2. (a) Interaction of a breather with an impurity for $\alpha = -0.52$, which corresponds to the impurity excitation case. (b) Evolution of the moving breather for $\alpha = -0.3$, which corresponds to the trapping case. The moving breather becomes trapped by the impurity; afterwards, the breather emits phonon radiation and its energy centre oscillates between the sites adjacent to the impurity.

neighbouring sites, as figure 2 shows. The trapped breather emits a great amount of phonon radiation and seems to be chaotic.

- *Well.* The impurity acts as a potential well. It occurs for $\alpha \in (\alpha_3, 0)$ and consists of an acceleration of the breather as it approaches to the impurity, and a deceleration after the impurity has been passed through.

4. Discussion

It is observed that the breather bifurcates with the zero solution at $\alpha = \alpha_{res}$. That is, for α smaller than this value, no impurity breather exists. At $\alpha = \alpha_{res}$, the frequency of the impurity mode coincides with the moving breather frequency, i.e., in (2), $\omega_{\mathrm{L}} = \omega_{\mathrm{b}}$.

The scenario for the trapped breathers when $\alpha < 0$ is the following: the impurity mode has $q = 0$, and also all the particles of the impurity breather vibrate in phase; this vibration pattern indicates that the impurity breather bifurcates from the impurity mode and it will be the only localized mode that exists when the impurity is excited for $\alpha > \alpha_{res}$. Thus, when the moving breather reaches the impurity, it can excite the impurity mode. For $\alpha < \alpha_{res}$, the moving breather is always reflected. In addition, the impurity breather does not exist. Therefore, there might be a connection between both facts, i.e., the existence of the impurity breather seems to be a necessary condition in order to obtain a trapped breather.

If $\alpha > 0$, the impurity mode has $q = \pi$ but the impurity breather's sites vibrate again in phase, that is, the impurity breather does not bifurcate from the impurity mode. There are two different localized excitations: the tails of the (linear) impurity mode and the impurity breather. Thus, if the moving breather reaches the impurity site, it will excite these localized excitations. Therefore, we conjecture that the existence of both linear localized entities at the same time may be the reason why the impurity is unable to trap the breather when $\alpha > 0$.

Trapping hypothesis: *The existence of an impurity breather for a given value of α is a necessary condition for the existence of trapped breathers. However, if there exists an impurity mode with a vibration pattern different from the impurity breather one's, the trapped breather does not to exist.*

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